

Carbazole-2-carbonitrile, 5,6,7,8-tetrahydro-1-methyl-
73771-63-8 | DTXSID50224153

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.04e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

Image not found

1,10-Phenanthroline

Measured: 1.49e-02

Predicted: 5.60e-03

Image not found

Etryptamine

Measured: 2.71e-03

Predicted: 5.31e-02

Image not found

N-(1-Naphthyl)ethylenediamine

Measured: 1.07e-02

Predicted: 9.11e-02

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1-Phenyl-2-thiourea

Measured: 1.62e-02

Predicted: 7.48e-02